JOURNAL OF COMPLEXITY 17, 795–814 (2001)
doi:10.1006/jcom.2001.0595, available online at http://www.idealibrary.com on IDEAL®

Quasi-random Simulation of Linear Kinetic Equations

Christian Lécot and Abdoul Koudiraty

Laboratoire de Mathématiques, Université de Savoie,
73376 Le Bourget-du-Lac cedex, France
E-mail: Christian.Lecot@univ-savoie.fr, Abdoul.Koudiraty@univ-savoie.fr

Received February 25, 2000; revised October 9, 2000; accepted October 20, 2000;
published online September 20, 2001

We study the improvement achieved by using quasi-random sequences in place of pseudo-random numbers for solving linear spatially homogeneous kinetic equations. Particles are sampled from the initial distribution. Time is discretized and

time step, the number order of the particles is scrambled according to their velocities. Convergence of the method is proved. Numerical results are presented for a sample problem in dimensions 1, 2 and 3. We show that by using quasi-random sequences in place of pseudo-random points, we are able to obtain reduced errors for the same number of particles. © 2001 Elsevier Science

1. INTRODUCTION

Kinetic equations provide mathematical models for the statistical evolution of particles. Applications can be found in the field of rarefied gas dynamics or semi-conductor devices. A distribution function $f(\mathbf{x}, \mathbf{v}, t)$, which represents the density of particles having position $\mathbf{x}$ and velocity $\mathbf{v}$ at time t, is solution of a non-stationary integro-differential equation. One method for approximating kinetic equations is random particle simulation [1, 11]. Particles are sampled from some known initial distribution. Random numbers are used to move the particles in phase space according to the dynamics described in the equation.

Monte Carlo methods are the only viable methods for a wide range of high-dimensional problems. They are easy to use, but the price for this

0885-064X/01 $35.00

simplicity is that Monte Carlo methods can be extremely slow. Consequently, even modest improvements can have substantial impact on the efficiency and range of applicability for Monte Carlo methods [2]. An approach to acceleration of the convergence rate is to change the choice of random numbers. Quasi-Monte Carlo methods use quasi-random (also known as low-discrepancy) sequences instead of random (or pseudo-random) [12, 15]. Today, low-discrepancy sequences are at the core of many simulations with improved convergence [16–18] and new research focuses on rationalizing these gains [19].

In this presentation we study the improvement achieved by using quasi-random sequences in place of pseudo-random numbers for solving the equation

$$\frac{\partial f}{\partial t}(\mathbf{v}, t) = \int_{\mathbf{R}^s} (f(\mathbf{v}', t)\, F(\mathbf{v}) - f(\mathbf{v}, t)\, F(\mathbf{v}'))\, \sigma(\mathbf{v}, \mathbf{v}')\, d\mathbf{v}', \tag{1a}$$

$$f(\mathbf{v}, 0) = f_0(\mathbf{v}), \tag{1b}$$

where

$$F(\mathbf{v}) := \frac{1}{\pi^{s/2}} \mathrm{e}^{-|\mathbf{v}|^2}, \qquad \int_{\mathbf{R}^s} F(\mathbf{v})\, d\mathbf{v} = 1,$$

denotes the normalized Maxwellian and σ denotes the collision cross section. The linear spatially homogeneous Boltzmann equation (1a) models the velocities of neutrons in a gas moderator [3] or the velocities of electrons in a semiconductor [8]. For the Monte Carlo simulation, N particles with velocities $\mathbf{v}_j^{(0)}$ are introduced at $t = 0$. Time is discretized into time-steps of duration Δt. In each time interval, random collisions are performed between the particles and the fixed Maxwellian background. Pseudo-random numbers are used to decide which particles collide and the outcome of the collisions.

The important role of the discrepancy in the quasi-Monte Carlo method is documented in [12, 15]. For a fixed dimension s we denote by $I^s := [0, 1)^s$ the s-dimensional unit cube and by λ_s the s-dimensional Lebesgue measure. For a set X of N points $\mathbf{x}_0, \ldots, \mathbf{x}_{N-1}$ in I^s, define for any subset E of I^s the *local discrepancy*

$$D_N(E, X) := \frac{1}{N} \sum_{0 \leqslant j < N} c_E(\mathbf{x}_j) - \lambda_s(E),$$

in which c_E is the characteristic function of E. The *star discrepancy* of the point set X is then defined by

$$D_N^*(X) := \sup_{J \in \mathscr{J}^*} |D_N(J, X)|,$$

in which $\mathscr{J}^*$ is the family of all subintervals of I^s of the form $\prod_{i=1}^s [0, \xi_i)$. For a sequence $X \subset I^s$, we write $D_N^*(X)$ for the star discrepancy of the first N terms of X. The most powerful current methods of constructing low-discrepancy point sets and sequences are based on the theory of (t, m, s)-nets and (t, s)-sequences. Fix an integer $b \geqslant 2$. An *elementary interval in base b* is an interval of the form

$$J = \prod_{i=1}^{s} \left[\frac{a_i}{b^{d_i}}, \frac{a_i + 1}{b^{d_i}} \right),$$

with integers $d_i \geqslant 0$ and $0 \leqslant a_i < b^{d_i}$ for $1 \leqslant i \leqslant s$. Let $0 \leqslant t \leqslant m$ be integers. A (t, m, s)-*net in base b* is a point set X of b^m points in I^s such that $D_N(J, X) = 0$ for every elementary interval J in base b with $\lambda_s(J) = b^{t-m}$. Let $t \geqslant 0$ be an integer. A sequence $\mathbf{x}_0, \mathbf{x}_1, \ldots$ of points in I^s is a (t, s)-*sequence in base b* if, for all integers $n \geqslant 0$ and $m > t$, the points $\mathbf{x}_j$ with $nb^m \leqslant j < (n+1)\, b^m$ form a (t, m, s)-net in base b. It is clear that smaller values of t mean stronger regularity properties. Explicit discrepancy bounds for (t, m, s)-nets and (t, s)-sequences can be found in [13]. In the present paper we give an application of (t, s)-sequences to the simulation of a model kinetic equation.

It is important to mention that if we just replace pseudo-random numbers by low discrepancy sequences, correlations between the quasi-random points used in successive time-steps would lead to biased and incorrect results. In [4] it is shown that low-discrepancy sequences are not suited for the simulation of stochastic differential equations. Here we use quasi-random points along with a renumbering technique to eliminate correlations. Between collisions, the number order of the particles is scrambled according to their velocities. The method is to first sort the particles into slabs, according to the first coordinate of their velocity. The particles of each slab are then sorted into boxes according to the second coordinate of their velocity, and so on. Similar techniques were used in applying quasi-random sequences to simulations for solving a one-dimensional nonlinear Boltzmann equation [5], a linear Boltzmann equation in the unit cube [6] or the heat equation [7, 9].

In Section 2 the quasi-random simulation and its basic properties are presented. Section 3 contains convergence results as to the number of particles tends to infinity. Finally, we present results from our solutions of a model problem in Section 4.

2. DISCRETE SIMULATION

We consider the linear kinetic equation (1a)–(1b), where the collision cross section is assumed to be nonnegative, symmetric and bounded, i.e.,

$$0 \leqslant \sigma(\mathbf{v}, \mathbf{v}') \leqslant \|\sigma\|_\infty < +\infty \qquad \text{and} \qquad \sigma(\mathbf{v}, \mathbf{v}') = \sigma(\mathbf{v}', \mathbf{v}).$$

The initial condition f_0 is assumed to satisfy

$$f_0(\mathbf{v}) \geqslant 0 \qquad \text{and} \qquad \int_{\mathbf{R}^s} f_0(\mathbf{v})\, d\mathbf{v} = 1.$$

The "mass" of the system is conserved by Eq. (1a):

$$\forall t > 0 \qquad \int_{\mathbf{R}^s} f(\mathbf{v}, t)\, d\mathbf{v} = 1. \tag{2}$$

A weak formulation of Eq. (1a) can be expressed as

$$\forall \chi \in \mathscr{C}(\mathbf{R}^s) \qquad \frac{d}{dt}\int_{\mathbf{R}^s} \chi(\mathbf{v})\, f(\mathbf{v}, t)\, d\mathbf{v}$$

$$= \int_{\mathbf{R}^{2s}} (\chi(\mathbf{v}') - \chi(\mathbf{v}))\, \sigma(\mathbf{v}, \mathbf{v}')\, f(\mathbf{v}, t)\, F(\mathbf{v}')\, d\mathbf{v}\, d\mathbf{v}', \tag{3}$$

where $\mathscr{C}(\mathbf{R}^s)$ denotes the set of all measurable characteristic functions on $\mathbf{R}^s$. We choose integers $b \geqslant 2$ and $d_1 \geqslant 0, \ldots, d_s \geqslant 0$. We set $m := d_1 + \cdots + d_s$ and $N := b^m$. The method consists in modelling trajectories (in the velocity space) of a particle system of the form

$$V(t) := \{\mathbf{v}_j(t) : 0 \leqslant j < N\}, \qquad t > 0. \tag{4}$$

The first step in the simulation is the approximation of the initial function f_0 by a system of particles

$$V^{(0)} := V(0) = \{\mathbf{v}_j^{(0)} : 0 \leqslant j < N\},$$

which are sampled from the measure $f_0(\mathbf{v})\, d\mathbf{v}$. The length Δt of the time-steps is chosen so that

$$\Delta t\, \|\sigma\|_\infty \leqslant 1. \tag{5}$$

We put

$$t_n := n\,\Delta t, \qquad f_n(\mathbf{v}) := f(\mathbf{v}, t_n).$$

For the evolution of the system (4) we use a sequence $X = \{\mathbf{x}_0, \mathbf{x}_1, \ldots\}$ of points which is a $(t, 2s+1)$-sequence in base b. Let

$$X^{(n)} := \{\mathbf{x}_{nN+j} : 0 \leqslant j < N\}.$$

We define the maps P' and P'' by

$$P' : \mathbf{x} = (x_1, \ldots, x_{2s+1}) \in I^{2s+1} \to \mathbf{x}' := (x_1, \ldots, x_s) \in I^s,$$
$$P'' : \mathbf{x} = (x_1, \ldots, x_{2s+1}) \in I^{2s+1} \to \mathbf{x}'' := (x_{s+1}, \ldots, x_{2s}) \in I^s$$

and we denote by $\mathring{I}$ the open unit interval. We assume

(H1) $P'X^{(n)}$ is a $(0, m, s)$-net in base b,
(H2) $P''X \subset \mathring{I}^s$.

Let

$$V^{(n)} := V(t_n) = \{\mathbf{v}_j^{(n)} : 0 \leqslant j < N\}.$$

The steps of the procedure of modelling a transition $V(t_n) \to V(t_{n+1})$ are as follows.

I. Relabeling: the particles are labeled anew using a multi-index $\mathbf{a} = (a_1, \ldots, a_s)$ with $0 \leqslant a_i < b^{d_i}$ for $1 \leqslant i \leqslant s$, so that

$$a_1 = b_1, \ldots, a_{i-1} = b_{i-1}, a_i < b_i \Rightarrow v_{\mathbf{a},i}^{(n)} \leqslant v_{\mathbf{b},i}^{(n)}.$$

See Fig. 1 in two dimensions.

II. Relaxation: let

$$f^{(n)}(\mathbf{v}) := \frac{1}{N} \sum_{0 \leqslant j < N} \delta(\mathbf{v} - \mathbf{v}_j^{(n)}),$$

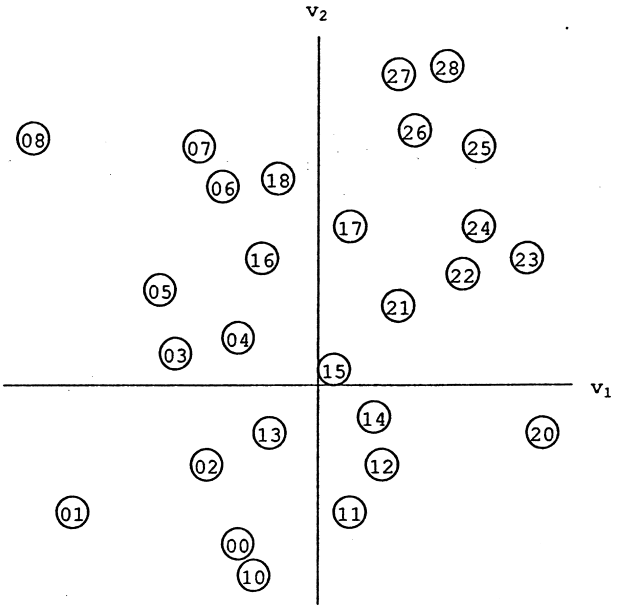

FIG. 1. Labeling the particles with a multi-index for $s = 2$, $b = 3$, $d_1 = 1$, $d_2 = 2$.

where δ denotes the Dirac mass. An approximation $g^{(n+1)}$ of the measure $f_{n+1}(\mathbf{v})\, d\mathbf{v}$ is defined using Eq. (3)

$$\frac{1}{\Delta t}\int_{\mathbf{R}^s} \chi(\mathbf{v})(g^{(n+1)}(\mathbf{v}) - f^{(n)}(\mathbf{v}))$$

$$= \int_{\mathbf{R}^{2s}} (\chi(\mathbf{v}') - \chi(\mathbf{v}))\, \sigma(\mathbf{v}, \mathbf{v}')\, f^{(n)}(\mathbf{v})\, F(\mathbf{v}')\, d\mathbf{v}'.$$

We find, for any $\chi \in \mathscr{C}(\mathbf{R}^s)$,

$$\int_{\mathbf{R}^s} \chi(\mathbf{v})\, g^{(n+1)}(\mathbf{v}) = \frac{1}{N}\sum_{\mathbf{a}} \left(1 - \Delta t \int_{\mathbf{R}^s} \sigma(\mathbf{v}_{\mathbf{a}}^{(n)}, \mathbf{v}')\, F(\mathbf{v}')\, d\mathbf{v}'\right) \chi(\mathbf{v}_{\mathbf{a}}^{(n)})$$

$$+ \frac{\Delta t}{N}\sum_{\mathbf{a}} \int_{\mathbf{R}^s} \chi(\mathbf{v}')\, \sigma(\mathbf{v}_{\mathbf{a}}^{(n)}, \mathbf{v}')\, F(\mathbf{v}')\, d\mathbf{v}'. \tag{6}$$

III. Integration: define

$$e(v) := \frac{1}{\sqrt{\pi}} \int_{-\infty}^{v} \mathrm{e}^{-w^2}\, dw, \qquad v \in \mathbf{R},$$
$$d(x) := e^{-1}(x), \qquad x \in \mathring{I},$$
$$d^{\otimes s}(\mathbf{x}) := (d(x_1), \ldots, d(x_s)), \qquad \mathbf{x} \in \mathring{I}^s.$$

From Eq. (6) we find that

$$\int_{\mathbf{R}^s} \chi(\mathbf{v})\, g^{(n+1)}(\mathbf{v}) = \frac{1}{N} \sum_{\mathbf{a}} (1 - \Delta t \int_{\mathring{I}^s} \sigma(\mathbf{v}_{\mathbf{a}}^{(n)}, d^{\otimes s}(\mathbf{x}''))\, d\mathbf{x}'')\, \chi(\mathbf{v}_{\mathbf{a}}^{(n)})$$
$$+ \frac{\Delta t}{N} \sum_{\mathbf{a}} \int_{\mathring{I}^s} \chi \circ d^{\otimes s}(\mathbf{x}'')\, \sigma(\mathbf{v}_{\mathbf{a}}^{(n)}, d^{\otimes s}(\mathbf{x}''))\, d\mathbf{x}''. \qquad (7)$$

Let $c_{\mathbf{a}}$ be the characteristic function of

$$I_{\mathbf{a}} := \prod_{i=1}^{s} \left[\frac{a_i}{b^{d_i}}, \frac{a_i + 1}{b^{d_i}} \right)$$

and $k_{\mathbf{a}}^{(n)}$ be the characteristic function of the set

$$\{\mathbf{x} = (\mathbf{x}', x_{s+1}) \in \mathring{I}^s \times I : x_{s+1} < \Delta t \sigma(\mathbf{v}_{\mathbf{a}}^{(n)}, d^{\otimes s}(\mathbf{x}'))\}.$$

To each $\chi \in \mathscr{C}(\mathbf{R}^s)$ there corresponds a characteristic function $C^{(n+1)}$ on $I^s \times \mathring{I}^s \times I$ by the formula

$$C^{(n+1)}(\mathbf{x}) := \sum_{\mathbf{a}} c_{\mathbf{a}}(\mathbf{x}')(1 - k_{\mathbf{a}}^{(n)}(\mathbf{x}'', x_{2s+1}))\, \chi(\mathbf{v}_{\mathbf{a}}^{(n)})$$
$$+ \sum_{\mathbf{a}} c_{\mathbf{a}}(\mathbf{x}')\, k_{\mathbf{a}}^{(n)}(\mathbf{x}'', x_{2s+1})\, \chi \circ d^{\otimes s}(\mathbf{x}''), \qquad (8)$$

for $\mathbf{x} = (\mathbf{x}', \mathbf{x}'', x_{2s+1})$. Then Eq. (7) can be written in a convenient form for quasi-Monte Carlo approximation

$$\int_{\mathbf{R}^s} \chi(\mathbf{v})\, g^{(n+1)}(\mathbf{v}) = \int_{I^s \times \mathring{I}^s \times I} C^{(n+1)}(\mathbf{x})\, d\mathbf{x}. \qquad (9)$$

The particle system $V^{(n+1)}$ at time t_{n+1} is then defined by

$$\forall \chi \in \mathscr{C}(\mathbf{R}^s) \qquad \int_{\mathbf{R}^s} \chi(\mathbf{v})\, f^{(n+1)}(\mathbf{v}) := \frac{1}{N} \sum_{0 \leqslant j < N} C^{(n+1)}(\mathbf{x}_{nN+j}).$$

Let $\lfloor x \rfloor$ denote the integer part of the value x. Define a function

$$\mathbf{a}(\mathbf{x}) := (\lfloor b^{d_1} x_1 \rfloor, \ldots, \lfloor b^{d_s}, x_s \rfloor), \qquad \mathbf{x} \in I^s.$$

Steps **II** and **III** can be summarized as follows:

• if $x_{nN+j,\,2s+1} < \Delta t \sigma(\mathbf{v}^{(n)}_{\mathbf{a}(\mathbf{x}'_{nN+j})}, d^{\otimes s}(\mathbf{x}''_{nN+j}))$, then the particle labeled $\mathbf{a}(\mathbf{x}'_{nN+j})$ collides with the Maxwellian background and its velocity becomes

$$\mathbf{v}^{(n+1)}_{\mathbf{a}(\mathbf{x}'_{nN+j})} = d^{\otimes s}(\mathbf{x}''_{nN+j}),$$

• if $x_{nN+j,\,2s+1} \geqslant \Delta t \sigma(\mathbf{v}^{(n)}_{\mathbf{a}(\mathbf{x}'_{nN+j})}, d^{\otimes s}(\mathbf{x}''_{nN+j}))$, then no colision occurs and the velocity of the particle labeled $\mathbf{a}(\mathbf{x}'_{nN+j})$ is unchanged

$$\mathbf{v}^{(n+1)}_{\mathbf{a}(\mathbf{x}'_{nN+j})} = \mathbf{v}^{(n)}_{\mathbf{a}(\mathbf{x}'_{nN+j})}.$$

3. CONVERGENCE

The justification of the quasi-random simulation is given in this section by showing convergence (as $N \to \infty$) of the measure $f^{(n)}(\mathbf{v})$ to the measure $f_n(\mathbf{v})\, d\mathbf{v}$. One may consider discrepancies for non-uniform distributions. Let

$$\rho\colon \mathbf{R}^s \to \mathbf{R}_+ \qquad \text{such that} \quad \int_{\mathbf{R}^s} \rho(\mathbf{v})\, d\mathbf{v} = 1.$$

For a set V of N points $\mathbf{v}_0, \ldots, \mathbf{v}_{N-1}$ in $\mathbf{R}^s$, define for any subset R of $\mathbf{R}^s$ the *local ρ-discrepancy*

$$D_N(R, V; \rho) := \frac{1}{N} \sum_{0 \leqslant j < N} \chi_R(\mathbf{v}_j) - \int_{\mathbf{R}^s} \chi_R(\mathbf{v})\, \rho(\mathbf{v})\, d\mathbf{v},$$

in which χ_R is the characteristic function of R. The *star ρ-discrepancy* of the point set V is defined by

$$D_N^*(V; \rho) := \sup_{\mathbf{w} \in \mathbf{R}^s} |D_N(R_\mathbf{w}, V; \rho)|,$$

in which $R_\mathbf{w} := \prod_{i=1}^s (-\infty, w_i)$. Let $\chi_\mathbf{w}$ denote the characteristic function of $R_\mathbf{w}$ and define

$$\chi_{\mathbf{w},1}(\mathbf{v}, \mathbf{v}') := \chi_\mathbf{w}(\mathbf{v}), \qquad \chi_{\mathbf{w},2}(\mathbf{v}, \mathbf{v}') := \chi_\mathbf{w}(\mathbf{v}'), \qquad \text{for} \quad \mathbf{v}, \mathbf{v}' \in \mathbf{R}^s.$$

We have the recurrence formula

$$D_N(R_\mathbf{w}, V^{(n+1)}; f_{n+1}) = D_N(R_\mathbf{w}, V^{(n)}; f_n) - \Delta t \varepsilon_\mathbf{w}^{(n)} + \Delta t\, \delta_\mathbf{w}^{(n)} + D_N(E_\mathbf{w}^{(n+1)}, X^{(n)}). \tag{10}$$

Here

$$\varepsilon_\mathbf{w}^{(n)} := \frac{1}{\Delta t} \int_{\mathbf{R}^s} \chi_\mathbf{w}(\mathbf{v})(f_{n+1}(\mathbf{v}) - f_n(\mathbf{v}))\, d\mathbf{v} - \int_{\mathbf{R}^{2s}} (\chi_\mathbf{w}(\mathbf{v}') - \chi_\mathbf{w}(\mathbf{v}))\, \sigma(\mathbf{v}, \mathbf{v}')\, F(\mathbf{v}')\, f_n(\mathbf{v})\, d\mathbf{v}\, d\mathbf{v}'$$

is the *truncation error* which is easily bounded:

$$|\varepsilon_\mathbf{w}^{(n)}| \leqslant \int_{t_n}^{t_{n+1}} \int_{\mathbf{R}^s} \left| \frac{\partial^2 f}{\partial t^2}(\mathbf{v}, t) \right| d\mathbf{v}\, dt. \tag{11}$$

The *error term*

$$\delta_\mathbf{w}^{(n)} := \int_{\mathbf{R}^{2s}} (\chi_\mathbf{w}(\mathbf{v}') - \chi_\mathbf{w}(\mathbf{v}))\, \sigma(\mathbf{v}, \mathbf{v}')\, F(\mathbf{v}')\, f^{(n)}(\mathbf{v})\, d\mathbf{v}' - \int_{\mathbf{R}^{2s}} (\chi_\mathbf{w}(\mathbf{v}') - \chi_\mathbf{w}(\mathbf{v}))\, \sigma(\mathbf{v}, \mathbf{v}')\, F(\mathbf{v}')\, f_n(\mathbf{v})\, d\mathbf{v}\, d\mathbf{v}'$$

can be written in the form $\delta_\mathbf{w}^{(n)} = -\delta_{\mathbf{w},1}^{(n)} + \delta_{\mathbf{w},2}^{(n)}$, where

$$\delta_{\mathbf{w},k}^{(n)} := \frac{1}{N} \sum_{0 \leqslant j < N} \Sigma_{\mathbf{w},k}(\mathbf{v}_j^{(n)}) - \int_{\mathbf{R}^s} \Sigma_{\mathbf{w},k}(\mathbf{v})\, f_n(\mathbf{v})\, d\mathbf{v}, \qquad k = 1, 2$$

and

$$\Sigma_{\mathbf{w},k}(\mathbf{v}) := \int_{\mathbf{R}^s} (\sigma\chi_{\mathbf{w},k})(\mathbf{v},\mathbf{v}')\, F(\mathbf{v}')\, d\mathbf{v}', \qquad \mathbf{v} \in \mathbf{R}^s.$$

The following result is an analogue of the Koksma–Hlawka inequality.

LEMMA 3.1. *Suppose ρ is a Riemann-integrable function on $\mathbf{R}^s$ such that $\rho \geqslant 0$ and $\int_{\mathbf{R}^s} \rho(\mathbf{v})\, d\mathbf{v} = 1$. Let f be a function on $\mathbf{R}^s$ such that f and $|f|$ are of bounded variation in the sense of Hardy and Krause. If f or ρ is continuous and if $\mathbf{v}_0, \ldots, \mathbf{v}_{N-1}$ are points in $\mathbf{R}^s$, then*

$$\left| \frac{1}{N} \sum_{0 \leqslant j < N} f(\mathbf{v}_j) - \int_{\mathbf{R}^s} f(\mathbf{v})\, \rho(\mathbf{v})\, d\mathbf{v} \right| \leqslant V(f)\, D_N^*(V; \rho).$$

Then we have an upper bound for the error term $\delta_{\mathbf{w}}^{(n)}$.

PROPOSITION 3.1. *If σ is of bounded variation $V(\sigma)$ on $\mathbf{R}^{2s}$ in the sense of Hardy and Krause and if f_n is a continuous function on $\mathbf{R}^s$, then*

$$|\delta_{\mathbf{w}}^{(n)}| \leqslant (2V(\sigma) + \|\sigma\|_\infty)\, D_N^*(V^{(n)}; f_n).$$

Proof. It follows from Lemma 3.1 that

$$|\delta_{\mathbf{w},k}^{(n)}| \leqslant V(\Sigma_{\mathbf{w},k})\, D_N^*(V^{(n)}; f_n), \qquad k = 1, 2.$$

Then, by an analogue of [6, Lemma 2], we obtain

$$V(\Sigma_{\mathbf{w},1}) \leqslant V(\sigma) + \|\sigma\|_\infty \qquad \text{and} \qquad V(\Sigma_{\mathbf{w},2}) \leqslant V(\sigma),$$

hence the result. ∎

Next, we present a bound for the *error of the quasi-Monte Carlo approximation* $D_N(E_{\mathbf{w}}^{(n+1)}, X^{(n)})$. Here

$$E_{\mathbf{w}}^{(n+1)} := \{\mathbf{x} \in I^s \times \overset{\circ}{I}{}^s \times I : C_{\mathbf{w}}^{(n+1)}(\mathbf{x}) = 1\},$$

where $C_{\mathbf{w}}^{(n+1)}$ corresponds to $\chi_{\mathbf{w}}$ by Formula (8). We split up $E_{\mathbf{w}}^{(n+1)}$ into the disjoint sets $G_{\mathbf{w}}^{(n)} \setminus F_{\mathbf{w},1}^{(n)}$ and $F_{\mathbf{w},2}^{(n)}$, where

$$G_{\mathbf{w}}^{(n)} := \{\mathbf{x} \in I^s \times \overset{\circ}{I}{}^s \times I : \sum_{\mathbf{a}} c_{\mathbf{a}}(\mathbf{x}')\, \chi_{\mathbf{w}}(\mathbf{v}_{\mathbf{a}}^{(n)}) = 1\},$$

$$F_{\mathbf{w},k}^{(n)} := \{\mathbf{x} \in I^s \times \overset{\circ}{I}{}^s \times I : x_{2s+1} < s_{\mathbf{w},k}^{(n)}(\mathbf{x}', \mathbf{x}'')\}, \qquad k = 1, 2$$

and

$$s^{(n)}_{\mathbf{w},k}(\mathbf{x}', \mathbf{x}'') := \Delta t \sum_{\mathbf{a}} c_{\mathbf{a}}(\mathbf{x}')(\sigma\chi_{\mathbf{w},k})(\mathbf{v}^{(n)}_{\mathbf{a}}, d^{\otimes s}(\mathbf{x}'')), \qquad (\mathbf{x}', \mathbf{x}'') \in I^s \times \overset{\circ}{I}{}^s.$$

Since $F^{(n)}_{\mathbf{w},1} \subset G^{(n)}_{\mathbf{w}}$, we obtain

$$D_N(E^{(n+1)}_{\mathbf{w}}, X^{(n)}) = D_N(F^{(n)}_{\mathbf{w},2}, X^{(n)}) + D_N(G^{(n)}_{\mathbf{w}}, X^{(n)}) - D_N(F^{(n)}_{\mathbf{w},1}, X^{(n)}). \tag{12}$$

The notation $\mathbf{v} < \mathbf{w}$ will mean that $v_i < w_i$ for every i. By Hypothesis (H2) we have

$$D_N(G^{(n)}_{\mathbf{w}}, X^{(n)}) = D_N(P'G^{(n)}_{\mathbf{w}}, P'X^{(n)}). \tag{13}$$

Note that $P'G^{(n)}_{\mathbf{w}}$ can be represented as the disjoint union of elementary intervals in base b:

$$P'G^{(n)}_{\mathbf{w}} = \bigcup_{\mathbf{v}^{(n)}_{\mathbf{a}} < \mathbf{w}} I_{\mathbf{a}}. \tag{14}$$

By Hypothesis (H1), $P'X^{(n)}$ is a $(0, m, s)$-net in base b, hence

$$D_N(G^{(n)}_{\mathbf{w}}, X^{(n)}) = 0. \tag{15}$$

The following Lemma is a modified version of an earlier result [6, Lemma 4].

LEMMA 3.2. *Let f be a function of bounded variation $V(f)$ on $\mathbf{R}^s$ in the sense of Hardy and Krause. Let*

$$-\infty = w_{0,1} \leqslant w_{1,1} \leqslant \cdots \leqslant w_{n_1,1} = +\infty,$$
$$-\infty = w_{a_1,0,2} \leqslant w_{a_1,1,2} \leqslant \cdots \leqslant w_{a_1,n_2,2} = +\infty, \qquad \text{for} \quad 0 \leqslant a_1 < n_1,$$
$$\cdots$$
$$-\infty = w_{\mathbf{a}',0,s} \leqslant w_{\mathbf{a}',1,s} \leqslant \cdots \leqslant w_{\mathbf{a}',n_s,s} = +\infty \quad \text{for } \mathbf{a}' = (a_1, \ldots, a_{s-1}),\ 0 \leqslant a_i < n_i$$

define partitions of $[-\infty, +\infty]$ into subintervals. For $\mathbf{a} = (a_1, \ldots, a_s)$ with integers a_i, $0 \leqslant a_i < n_i$, let

$$R_{\mathbf{a}} := [w_{a_1,1}, w_{a_1+1,1}] \times [w_{a_1,a_2,2}, w_{a_1,a_2+1,2}] \times \cdots \times [w_{\mathbf{a}',a_s,s}, w_{\mathbf{a}',a_s+1,s}]$$

and $\mathbf{u}_\mathbf{a}$, $\mathbf{v}_\mathbf{a} \in R_\mathbf{a}$. *Then*

$$\sum_{\mathbf{a}} |f(\mathbf{v}_\mathbf{a}) - f(\mathbf{u}_\mathbf{a})| \leqslant V(f) \prod_{i=1}^{s} n_i \sum_{i=1}^{s} \frac{1}{n_i}.$$

We are now in a position to prove an upper bound for $|D_N(F^{(n)}_{\mathbf{w},k}, X^{(n)})|$.

PROPOSITION 3.2. *If σ is of bounded variation $V(\sigma)$ on $\mathbf{R}^{2s}$ in the sense of Hardy and Krause, then, for $k = 1, 2$,*

$$|D_N(F^{(n)}_{\mathbf{w},k}, X^{(n)})| \leqslant \frac{1}{b^{d_s - t - (s+1)\lfloor (d_s - t)/(s+2) \rfloor}} + \Delta t (V(\sigma) + \|\sigma\|_\infty) \left(\sum_{i=1}^{s-1} \frac{1}{b^{d_i}} + \frac{s+1}{b^{\lfloor (d_s - t)/(s+2) \rfloor}} \right).$$

Proof. We may replace $F^{(n)}_{\mathbf{w},k}$ by

$$\tilde{F}^{(n)}_{\mathbf{w},k} := \{\mathbf{x} \in I^{2s+1} : x_{2s+1} < s^{(n)}_{\mathbf{w},k}(\mathbf{x}', \mathbf{x}'')\}.$$

Let $\delta_1, \ldots, \delta_{2s}$ be integers. For $\boldsymbol{\alpha} = (\boldsymbol{\alpha}', \boldsymbol{\alpha}'')$, $\boldsymbol{\alpha}' := (\alpha_1, \ldots, \alpha_s)$, $\boldsymbol{\alpha}'' := (\alpha_{s+1}, \ldots, \alpha_{2s})$ with integers $0 \leqslant \alpha_i < b^{\delta_i}$ we put

$$I'_{\boldsymbol{\alpha}'} := \prod_{i=1}^{s} \left[\frac{\alpha_i}{b^{\delta_i}}, \frac{\alpha_i + 1}{b^{\delta_i}} \right), \qquad I''_{\boldsymbol{\alpha}''} := \prod_{i=s+1}^{2s} \left[\frac{\alpha_i}{b^{\delta_i}}, \frac{\alpha_i + 1}{b^{\delta_i}} \right), \qquad J_{\boldsymbol{\alpha}} := I'_{\boldsymbol{\alpha}'} \times I''_{\boldsymbol{\alpha}''}$$

and, for $k = 1, 2$,

$$\underline{F}^{(n)}_{\mathbf{w},k} = \bigcup_{\boldsymbol{\alpha}} J_{\boldsymbol{\alpha}} \times [0, \inf_{J_{\boldsymbol{\alpha}}} s^{(n)}_{\mathbf{w},k}), \qquad \bar{F}^{(n)}_{\mathbf{w},k} = \bigcup_{\boldsymbol{\alpha}} J_{\boldsymbol{\alpha}} \times [0, \sup_{J_{\boldsymbol{\alpha}}} s^{(n)}_{\mathbf{w},k}),$$

$$\partial F^{(n)}_{\mathbf{w},k} = \bigcup_{\boldsymbol{\alpha}} J_{\boldsymbol{\alpha}} \times [\inf_{J_{\boldsymbol{\alpha}}} s^{(n)}_{\mathbf{w},k}, \sup_{J_{\boldsymbol{\alpha}}} s^{(n)}_{\mathbf{w},k}].$$

We have $\underline{F}^{(n)}_{\mathbf{w},k} \subset \tilde{F}^{(n)}_{\mathbf{w},k} \subset \bar{F}^{(n)}_{\mathbf{w},k}$ and $\bar{F}^{(n)}_{\mathbf{w},k} \setminus \underline{F}^{(n)}_{\mathbf{w},k} \subset \partial F^{(n)}_{\mathbf{w},k}$; hence

$$D_N(\underline{F}^{(n)}_{\mathbf{w},k}, X^{(n)}) - \lambda_{2s+1}(\partial F^{(n)}_{\mathbf{w},k}) \leqslant D_n(\tilde{F}^{(n)}_{\mathbf{w},k}, X^{(n)}) \leqslant D_N(\bar{F}^{(n)}_{\mathbf{w},k}, X^{(n)}) + \lambda_{2s+1}(\partial F^{(n)}_{\mathbf{w},k}).$$

A well-known bound [13, Lemma 3.4] yields

$$\max(|D_N(\underline{F}^{(n)}_{\mathbf{w},k}, X^{(n)})|, |D_N(\bar{F}^{(n)}_{\mathbf{w},k}, X^{(n)})|) \leqslant b^{\delta_1+\cdots+\delta_{2s}+t-m}$$

and so

$$|D_N(F^{(n)}_{\mathbf{w},k}, X^{(n)})| \leqslant \frac{b^{\delta_1+\cdots+\delta_{2s}}}{b^{m-t}} + \frac{1}{b^{\delta_1+\cdots+\delta_{2s}}} \sum_{\alpha} (\sup_{J_\alpha} s^{(n)}_{\mathbf{w},k} - \inf_{J_\alpha} s^{(n)}_{\mathbf{w},k}).$$

If $\delta_1 = d_1, \ldots, \delta_{s-1} = d_{s-1}$ and $\delta_s \leqslant d_s$, then

$$\sup_{J_\alpha} s^{(n)}_{\mathbf{w},k} = \Delta t \sup \{(\sigma\chi_{\mathbf{w},k})(\mathbf{v}^{(n)}_{\alpha_1,\ldots,\alpha_{s-1},a_s}, d^{\otimes s}(\mathbf{x}'')):$$
$$\alpha_s b^{d_s-\delta_s} \leqslant a_s < (\alpha_s+1)\, b^{d_s-\delta_s}, \mathbf{x}'' \in I''_{\alpha''}\}.$$

A similar statement holds for $\inf_{J_\alpha} s^{(n)}_{\mathbf{w},k}$. Because the velocities $\mathbf{v}^{(n)}_{\mathbf{a}}$ are ordered so that

$$a_1 = b_1, \ldots, a_{i-1} = b_{i-1}, a_i < b_i \Rightarrow v^{(n)}_{\mathbf{a},i} \leqslant v^{(n)}_{\mathbf{b},i},$$

we can define partitions of $[-\infty, +\infty]$

$$-\infty = w^{(n)}_{0,1} \leqslant w^{(n)}_{1,1} \leqslant \cdots \leqslant w^{(n)}_{b^{\delta_1},1} = +\infty,$$
$$-\infty = w^{(n)}_{\alpha_1,0,2} \leqslant w^{(n)}_{\alpha_1,1,2} \leqslant \cdots \leqslant w^{(n)}_{\alpha_1,b^{\delta_2},2} = +\infty, \qquad \text{for} \quad 0 \leqslant \alpha_1 < b^{\delta_i},$$
$$-\infty = w^{(n)}_{\alpha_1,\ldots,\alpha_{s-1},0,s} \leqslant w^{(n)}_{\alpha_1,\ldots,\alpha_{s-1},1,s} \leqslant \cdots \leqslant w^{(n)}_{\alpha_1,\ldots,\alpha_{s-1},b^{\delta_s},s} = +\infty,$$
$$\text{for} \quad 0 \leqslant \alpha_1 < b^{\delta_1}, \ldots, 0 \leqslant \alpha_{s-1} < b^{\delta_{s-1}}$$

such that, for any integer a_s with $\alpha_s b^{d_s-\delta_s} \leqslant a_s < (\alpha_s+1)\, b^{d_s-\delta_s}$, we have

$$\mathbf{v}^{(n)}_{\alpha_1,\ldots,\alpha_{s-1},a_s} \in [w^{(n)}_{\alpha_1,1}, w^{(n)}_{\alpha_1+1,1}] \times \cdots \times [w^{(n)}_{\alpha_1,\ldots,\alpha_s,s}, w^{(n)}_{\alpha_1,\ldots,\alpha_s+1,s}].$$

It follows then from Lemma 3.2 that

$$\sum_{\alpha} (\sup_{J_\alpha} s^{(n)}_{\mathbf{w},k} - \inf_{J_\alpha} s^{(n)}_{\mathbf{w},k}) \leqslant \Delta t(V(\sigma)+\|\sigma\|_\infty)\, b^{\delta_1+\cdots+\delta_{2s}} \sum_{i=1}^{2s} \frac{1}{b^{\delta_i}}.$$

By choosing $\delta_s = \cdots = \delta_{2s} = \lfloor (d_s - t)/(s+2) \rfloor$, we complete the proof. ∎

We can combine the previous bounds to derive an upper bound for the error of the scheme. We put $|\sigma| := 2V(\sigma) + \|\sigma\|_\infty$.

PROPOSITION 3.3. *If σ is of bounded variation $V(\sigma)$ on $\mathbf{R}^{2s}$ in the sense of Hardy and Krause, then*

$$\begin{aligned} D_N^*(V^{(n)}; f_n) \leqslant\ & e^{|\sigma| t_n} D_N^*(V^{(0)}; f_0) \\ & + \Delta t \int_0^{t_n} \int_{\mathbf{R}^s} e^{|\sigma|(t_n - t)} \left| \frac{\partial^2 f}{\partial t^2}(\mathbf{v}, t) \right| d\mathbf{v}\, dt \\ & + \frac{2e^{|\sigma| t_n}}{|\sigma| \Delta t} \left(\frac{1}{b^{d_s - t - (s+1)\lfloor (d_s - t)/(s+2) \rfloor}} \right. \\ & \left. + \Delta t (V(\sigma) + \|\sigma\|_\infty) \left(\sum_{i=1}^{s-1} \frac{1}{b^{d_i}} + \frac{s+1}{b^{\lfloor (d_s - t)/(s+2) \rfloor}} \right) \right). \end{aligned}$$

4. NUMERICAL EXPERIMENTS

In this section we present the results of numerical simulations according to the method described in Section 2. Our model problem is very simple, yet it is useful for studying the effect of the dimension s on the rate of convergence of the simulation. If the collision cross section σ is assumed to be constant, then Eq. (1a)–(1b) is an ordinary differential equation with solution

$$f(\mathbf{v}, t) = e^{-\sigma t} f_0(\mathbf{v}) + (1 + e^{-\sigma t}) F(\mathbf{v}). \tag{16}$$

We choose $\sigma = 1$ with the following initial data

$$f_0(\mathbf{v}) = \frac{2}{s} \left(\frac{1}{\pi} \right)^{s/2} |\mathbf{v}|^2 e^{-|\mathbf{v}|^2}$$

and we simulate the solution over the time interval $[0, 4.0]$. Pseudo-random (PR) simulations using pseudo-random numbers without relabeling are compared with quasi-random (QR) simulations. We use the (t, s)-sequences of Niederreiter [14], with small values of t. By [13, Corollary 5.17] a $(0, s)$-sequence in base b can only exist if $s \leqslant b$. Consequently (H1) is satisfied only if $b \geqslant s$.

Let $B(0, r)$ denote the ball $\{\mathbf{v} \in \mathbf{R}^s : |\mathbf{v}| < r\}$. For all the simulations the system $V^{(0)}$ is computed by mapping the $(0, m, s)$-net $P'X^{(0)}$ to $\mathbf{R}^s$ using the inverse function of

- $F_0(v) := \int_{-\infty}^{v} f_0(u)\, du$, if $s = 1$,
- $F_0(r) := \int_{B(0,r)} f_0(\mathbf{v})\, d\mathbf{v}$, if $s > 1$.

When $s > 1$, the computation of the discrepancy would be too expensive: the error of the simulation is measured by the *radial discrepancy*:

$$D_N^{(r)}(V^{(n)}; f_n) := \sup_{r>0} |D_N(B(0, r), V^{(n)}; f_n)|.$$

In order to estimate the rate of convergence of each simulation, a calculation with P time steps is performed and the *averaged error*

$$D_N := \frac{1}{P+1} \sum_{0 \leqslant n \leqslant P} D_N^{(r)}(V^{(n)}; f_n)$$

is computed. If one expects $D_N = \alpha N^{-\beta}$, one can estimate α and β by a linear fit to plots of $\log D_N$ versus $\log N$.

A more common practice is to measure the error in some scalar quantities, such as the first moments of the distribution. Here

$$M_{1,i}(f)(t) := \int_{\mathbf{R}^s} v_i f(\mathbf{v}, t)\, d\mathbf{v} = 0, \tag{17a}$$

$$M_2(f)(t) := \int_{\mathbf{R}^s} |\mathbf{v}|^2 f(\mathbf{v}, t)\, d\mathbf{v} = e^{-\sigma t} + \frac{s}{2}. \tag{17b}$$

In every time step let

$$e_{1,N}^{(n)} := \max_{1 \leqslant i \leqslant s} \left| \frac{1}{N} \sum_{0 \leqslant j < N} v_{j,i}^{(n)} - M_{1,i}(f)(t_n) \right|,$$

$$e_{2,N}^{(n)} := \left| \frac{1}{N} \sum_{0 \leqslant j < N} |\mathbf{v}_j^{(n)}|^2 - M_2(f)(t_n) \right|.$$

When a calculation with P time steps is performed, we compute the *moment errors*

$$E1_N := \frac{1}{P+1} \sum_{0 \leqslant n \leqslant P} e_{1,N}^{(n)} \quad \text{and} \quad E2_N := \frac{1}{P+1} \sum_{0 \leqslant n \leqslant P} e_{2,N}^{(n)}.$$

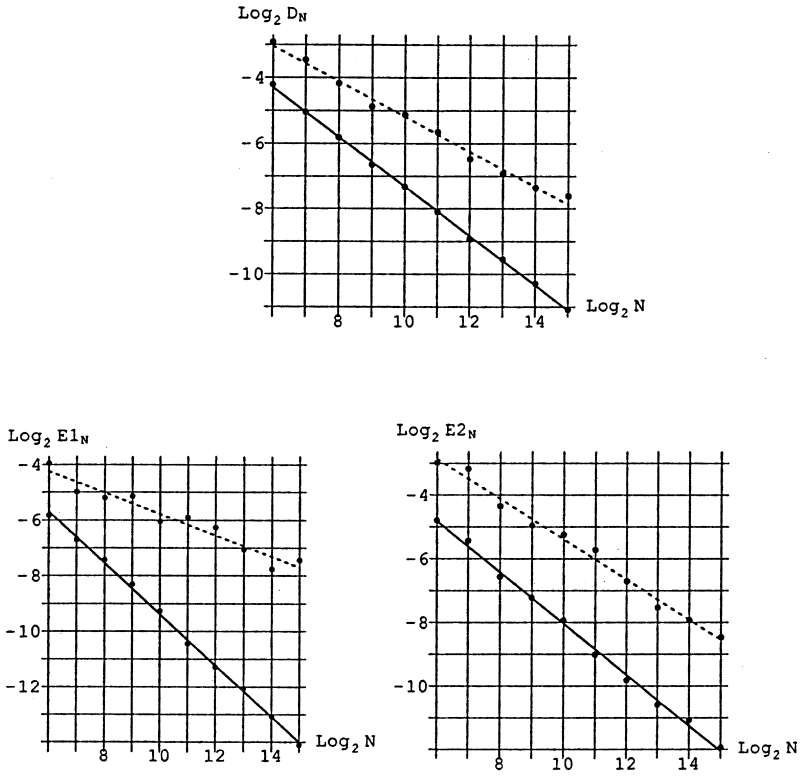

FIG. 2. Dimension $s = 1$. Linear fits to the errors: PR (dashed) vs. QR (solid) simulations. Top panel shows averaged errors. Bottom panels show first moment (left) and second moment (right) errors.

In dimension $s = 1$ a time step of $\Delta t = 0.001$ was chosen, so $P = 4,000$. The Niederreiter sequence in base 2 was used for the QR simulation. A comparison of the PR and QR simulations is shown in Fig. 2. The QR simulations clearly outperform the PR simulations in this case. One finds

$$D_N(\mathrm{PR}) \approx \frac{1.14}{N^{0.54}} \qquad \text{and} \qquad D_N(\mathrm{QR}) \approx \frac{1.19}{N^{0.76}}. \tag{18}$$

In dimension $s = 2$ we used $\Delta t = 0.002$, so $P = 2,000$. The Niederreiter sequence in base 3 was used for the QR simulation. In Fig. 3 we graph the error from solving the model problem using PR and QR simulations. Once

again, the QR simulations produce lower error and better convergence rate than the PR simulations. One has

$$D_N(\mathrm{PR}) \approx \frac{0.87}{N^{0.51}} \qquad \text{and} \qquad D_N(\mathrm{QR}) \approx \frac{1.23}{N^{0.63}}. \tag{19}$$

A further experiment was run to solve the model kinetic equation in dimension $s = 3$. The time-step was taken to be $\Delta t = 0.004$, so $P = 1,000$. The problem was implemented using the Niederreiter sequence in base 5 for the QR simulation. Figure 4 compares errors obtained in solving the model problem using PR and QR simulations. The quasi-random sequence shows a behavior which is better than the pseudo-random behavior, but

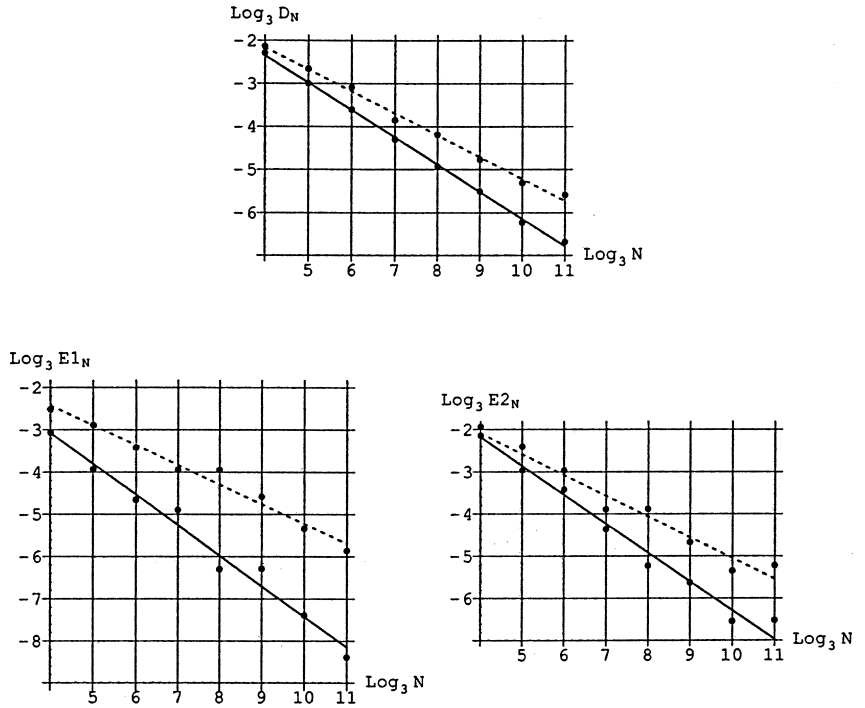

FIG. 3. Dimension $s = 2$. Linear fits to the errors: PR (dashed) vs. QR (solid) simulations. Top panel shows averaged errors. Bottom panels show first moment (left) and second moment (right) errors.

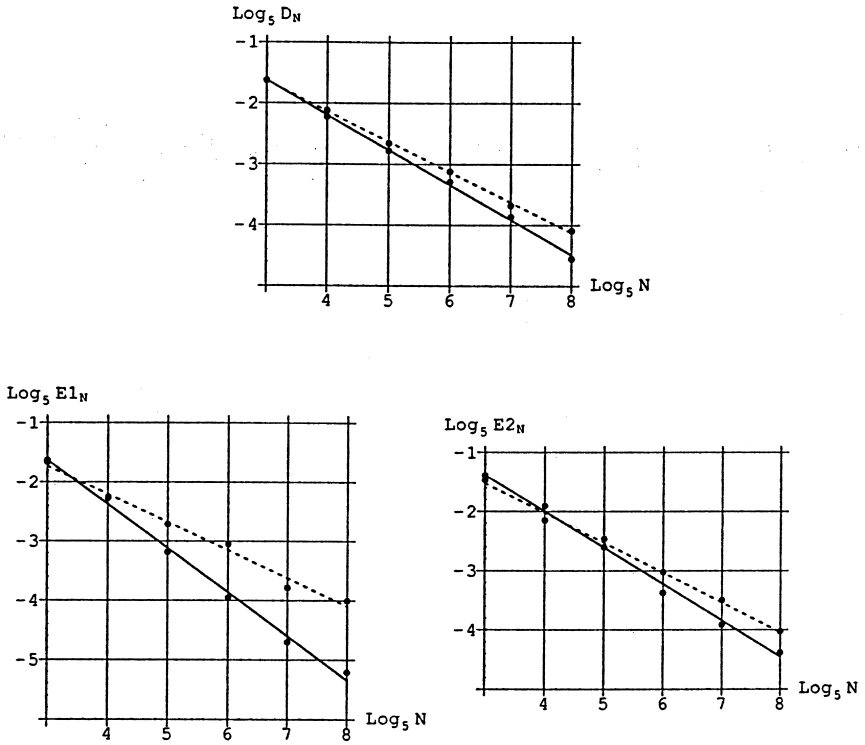

FIG. 4. Dimension $s = 3$. Linear fits to the errors: PR (dashed) vs. QR (solid) simulations. Top panel shows averaged errors. Bottom panels show first moment (left) and second moment (right) errors.

the level of improvement is less impressive than in lower dimensions. One obtains

$$D_N(\mathrm{PR}) \approx \frac{0.81}{N^{0.50}} \qquad \text{and} \qquad D_N(\mathrm{QR}) \approx \frac{1.18}{N^{0.57}}. \tag{20}$$

The results of the numerical experiments show that the upper bound of Proposition 3.3 is pessimistic.

5. CONCLUSION

We studied a quasi-random particle method for solving linear kinetic equations. The main feature of the method is the use of low-discrepancy

sequences for simulating collisions of the particles with the Maxwellian background. A key element in successfully applying the quasi-random sequences is a technique involving renumbering the particles after each time step. Convergence of the simulation as the number of particles increases has been proved. Computations were performed for a model kinetic equation, for which the exact solution is known, since in this case it is possible to compare the errors of the quasi-random simulation with the errors obtained when all decisions make use of pseudo-random methods, i.e., conventional Monte Carlo. It was shown that quasi-random simulation of simple linear kinetic equations can produce more accurate results for a given number of particles than pseudo-random simulation. Our computations also indicate that the error reduction for quasi-Monte Carlo is limited as the dimension increases, in a way very similar to the behavior of the error for quasi-Monte Carlo evaluation of integrals [10].

ACKNOWLEDGMENTS

The numerical experiments were carried out on a Fujitsu VPP-5000 computer, located at the CGCV-CEA (Centre Grenoblois de Calcul Vectoriel du Commissariat à l'Énergie Atomique). CGCV-CEA's support is greatly appreciated.

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